International Journal of Quantum Chemistry Author Index—Volume 73

Akpinar, S. See Bulut, N., 425

Alagona, G.

—; Ghio, C.; Monti, S.: Ab Initio Study of Preferential Interactions Between Aromatic Side Chains, 175

See Osman, R., 59

Angulo, J. C.

—; Romera, E.: Erratum to "Improved Upper Bounds for the Atomic Ionization Potential," 511

Åqvist, J. See Kolmodin, K., 147

Barone, V. See Rega, N., 219

Basosi, R. See Pogni, R., 249

Bastos, M. See Henriques, E. S., 237

Bertrand, P. See De Gioia, L., 187

Bhattacharyya, S. P. See Mondal, C. K., 469

Blaney, F. E.

Homology Modelling and Ab Initio Calculations Identify a Basis for Ligand Selectivity for the PPARγ Nuclear Hormone Receptor, 97

Blomberg, M. R. A. See Pavlov, M., 197

Boczar, M. See Wójcik, M. J., 275

Bouzida, D.

—; Rejto, P. A.; Verkhivker, G. M.: Monte Carlo Study of Ligand–Protein Binding Energy Landscapes with Weighted Histogram Analysis Method, 113

Bulut, N.

—; Yildiz, A.; Göğtaş, F.; Akpinar, S.: Quantum Wave Packet Study of $O(^1D) + HCl(v) \rightarrow ClO(v') + H$ Reaction, 425

Busi, E. See Pogni, R., 249

Cai, Z. See Tang, A., 505

Carloni, P. See Rothlisberger, U., 209

Casanova, M. See Magnasco, V., 333

Chaudhury, P. See Mondal, C. K., 469

Chen, C.

—; Shyu, S.-F.: Theoretical Study of Single-Bonded Nitrogen Cluster-Type Molecules, 349

Chen, J.-Q.

—; Xin, X.-J.; Fan, P.-D.; Ping, J.-L.: Algebraic Expressions of Irreducible Bases for Molecules $C_{20}H_{20}$, C_{80}, and C_{240}, 283

Chen, X.-Y.

—; Wu, T.; Ju, Q.; Ma, J.; Ju, G.-Z.: Theoretical Study of Reactions Between $AlH(^1\Sigma)$ and HF Molecule, 417

Cheranovskii, V. O.

—; Ezerskaya, E. V.; Zhikol, O. A.; Kinal, A.; Pamuk, H. O.: Effect of Doping on the Ground-State Spin of Stacked Organometallic Ferromagnets, 511

Chiu, L.-Y. C.

—; Moharerrzadeh, M.: Fourier Transform of Spherical Laguerre Gaussian Functions and Its Application in Molecular Integrals, 265

Ciarkowski, J. See Czaplewski, C., 61

Cimiraglia, R. See Zaitsevskii, A., 395

Cossi, M. See Rega, N., 219

Cotecchia, S. See Fanelli, F., 71

Czaplewski, C.

—; Pasenkiewicz-Gierual, M.; Ciarkowski, J.: G Protein-Coupled Receptor–Bioligand Interactions Modeled in a Phospholipid Bilayer, 61

De Benedetti, P. G. See Fanelli, F., 71

De Gioia, L.

—; Fantucci, P.; Guigliarelli, B.; Bertrand, P.: Ab Initio Investigation of the Structural and Electronic Differences Between Active-Site Models of [NiFe] and [NiFeSe] Hydrogenases, 187

Dehareng, D. See Dive, G., 161

Della Lunga, G. See Pogni, R., 249

Dive, G.

—; Dehareng, D.: Serine Peptidase Catalytic Machinery: Cooperative One-Step Mechanism, 161

Ezerskaya, E. V. See Cheranovskii, V. O., 511

Faglioni, F.

Goddard III, W. A.: GVB–RP: A Reliable MCSCF Wave Function for Large Systems, 1

Fakhreddine, K.

—; Kobeissi, H.; Korek, M.: Bound States of the Coupled-Channel Schrödinger Equation: General Eigenvalue Function, 325

Fan, P.-D. See Chen, J.-Q., 283

Fanelli, F.

—; Menziani, C.; Scheer, A.; Cotecchia, S.; De Benedetti, P. G.: Theoretical Study on Receptor–G Protein Recognition: New Insights into the Mechanism of the α1b-Adrenergic Receptor Activation, 71

Fantucci, P. See De Gioia, L., 187

Feng, J. See Tang, A., 505

Ferenczy, G. G. See Wu, P. H., 229

Fernández, N. See Nilsson, A. M., 85

Francisco, J. S.
An Ab Initio Study of the Structures and Energetics of CH_3OCl and CH_3ClO, 29

Geraldes, C. F. G. C. See Henriques, E. S., 237
Ghio, C. See Alagona, G., 175
See Osman, R., 59
Ghosh, D. K. See Sarma, C. R., 389
Gkoutos, G. See Nilsson, A. M., 85
Goddard III, W. A. See Faglioni, F., 1
Gögtaş, F. See Bulut, N., 425
Guigliarelli, B. See De Gioia, L., 187
Gunn, J. R. See Wang, Y., 357
Gutowski, M.
Favorable Performance of the DFT Methods in Predicting the Minimum-Energy Sructure of the Lowest Triplet State of WF_4, 369

Hadfield, A. T.
—; Mulholland, A. J.: Active-Site Dynamics of ASADH—A Bacterial Biosynethetic Enzyme, 137
Henriques, E. S.
—; Bastos, M.; Geraldes, C. F. G. C.; Ramos, M. J.: Computational Approaches to the Study of Some Lanthanide (III)–Polyazamacrocyclic Chelates for Magnetic Resonance Imaging, 237
Huang, L.
—; Massa, L.; Karle, J.: Quantum Crystallography Applied to Crystalline Maleic Anhydride, 439

Jaskólski, W. See Planelles, J., 341
Ju, G.-Z. See Chen, X.-Y., 417
Ju, Q. See Chen, X.-Y., 417
Jursic, B. S.
High Level of Ab Initio and Density Functional Theory Evalution of the C—O Bond Dissociation Energies in the Dimethyl Ether Anion, 299
Hybrid Density Functional Theory Study of Hydrogen Cluster Aromaticity by Computing Their Relative Energies and Magnetic Properties, 451

Kadolkar, C. Y. See Sarma, C. R., 389
Karle, J. See Huang, L., 439
Karwowski, J. See Planelles, J., 341
Keserű, G. M.
—; Kolossváry, I.; Székely, I.: Inhibitors of Cytochrome P450 Catalyzed Insecticide Metabolism: A Rational Approach, 123
Khan, A. A. See Kumar, A., 307
Kinal, A. See Cheranovskii, V. O., 511
Kobeissi, H. See Fakhreddine, K., 325
Kolmodin, K.
—; Åqvist, J.: Computational Modeling of Catalysis and Binding in Low-Molecular-Weight Protein Tyrosine Phosphatase, 147
Kolossváry, I. See Keserű, G. M., 123
Korek, M. See Fakhreddine, K., 325
Kumar, A.
—; Saha, B. C.; Khan, A. A.; Kumar, V.; Verma, S. K.; Prasad, K. K.: Depopulation of Low-Rydberg Na Atom in Collisions with Rare Gases: A Molecular-State Treatment, 307
Kumar, V. See Kumar, A., 307

La Cour Jansen, T.
—; Rettrup, S.; Sarma, C. R.; Snijders, J. G.; Palmieri, P.: On the Evaluation of Spin–Orbit Coupling Matrix Elements in a Spin-Adapted Basis, 23
Lü, X.
—; Xu, X.; Wang, N.; Zhang, Q.: Convergence from Clusters to the Bulk Solid: Ab Initio Calculations of $(MgO)_x$ ($x = 2 - 16$) Clusters, 377

Ma, J. See Chen, X.-Y., 417
Magnasco, V.
—; Rapallo, A.; Casanova, M.: New Translation Method for STOs and Its Application to Calculation of Overlap Integrals, 333
Massa, L. See Huang, L., 439
Mendizabal, F.
Theoretical Study of the Au–Ethylene Interaction, 317
Menziani, C. See Fanelli, F., 71
Micha, D. A.
Review of *Exploring Aspects of Computational Chemistry*, by J-M. Andre, D. H. Mosley, M-C. Andre, B. Champagne, E. Clementi, J. G. Fripiat, L. Leherte, L. Pisani, D. P. Vercauteren, and M. Vracko, 387
Moc, J.
On the Kinetic Stability of the SH_3X Species with X = F, Cl, 37
Moharerrzadeh, M. See Chiu, L.-Y. C., 265
Mondal, C. K.
—; Chaudhury, P.; Bhattacharyya, S. P.: Modeling Quantum Dynamics of Photodetachment from Closed-Shell Anions: Static versus Fluctuating Well-Depth Models, 469
Monti, S. See Alagona, G., 175
Mulholland, A. J. See Hadfield, A. T., 137

Nilsson, A. M.
—; Wijaywardene, M.; Gkoutos, G.; Wilson, K. M.; Fernández, N.; Reynolds, C. A.: Correlated Mutations in the HLA Class II Molecule, 85

Osman, R.
—; Alagona, G.; Ghio, C.: Introduction to Proceedings of the ISQBP President's Meeting: Molecular Structure and Dynamics in Biology (Biophysics Quarterly), 59

Palmieri, P. See La Cour Jansen, T., 23
Pamuk, H. O. See Cheranovskii, V. O., 511
Pan, Y. See Tang, A., 505

Pasenkiewicz-Gierula, M. See Czaplewski, C., 61
Pavlov, M.
—; Blomberg, M. R. A.; Siegbahn, P. E. M.: New Aspects of H_2 Activation by Nickel–Iron Hydrogenase, 197
Ping, J.-L. See Chen, J.-Q., 283
Planelles, J.
—; Karwowski, J.; Jaskólski, W.: Adaptation of One-Electron Basis Sets to Spatial Confinements, 341
Pogni, R.
—; Della Lunga, G.; Busi, E.; Basosi, R.: Lineshape Analysis of Heme-Protein-Derived Radicals Based on Simulation of EPR Spectra, 249
Pomelli, C. S. See Rega, N., 219
Prasad, K. K. See Kumar, A., 307

Ramos, M. J. See Henriques, E. S., 237
Rapallo, A. See Magnasco, V., 333
Rega, N.
—; Cossi, M.; Barone, V.; Pomelli, C. S.; Tomasi, J.: Toward an Effective and Reliable Representation of Solvent Effects in the Study of Biochemical Systems, 219
Rejto, P. A. See Bouzida, D., 113
Rettrup, S. See La Cour Jansen, T., 23
Reynolds, C. A. See Nilsson, A. M., 85
See Wu, P. H., 229
Rothlisberger, U.
—; Carloni, P.: Ab Initio Molecular Dynamics Studies of a Synthetic Biomimetic Model of Galactose Oxidase, 209
Roychoudhury, R. See Sinha, A., 497

Saha, B. C. See Kumar, A., 307
Sarma, C. R.
—; Ghosh, D. K.; Kadolkar, C. Y.: Graphical Approach to Correlations in High-Spin Systems, 389
See La Cour Jansen, T., 23
Scheer, A. See Fanelli, F., 71
Shang, Z. See Tang, A., 505
Shyu, S.-F. See Chen, C., 349
Siegbahn, P. E. M. See Pavlov, M., 197
Simonson, T.
Dielectric Relaxation in Proteins: Microscopic and Macroscopic Models, 45
Simos, T. E.
High Algebraic Order Explicit Methods with Reduced Phase-Lag for an Efficient Solution of the Schrödinger Equation, 479
Sinha, A.
—; Roychoudhury, R.: WKB and MAF Quantization Rules for Spatially Confined Quantum Mechanical Systems, 497
Smit, M. J.
Multicenter Integrals over Polarization Potential Operators, 403
Snijders, J. G. See La Cour Jansen, T., 23
Stoma, M. See Wójcik, M. J., 275
Székely, I. See Keserű, G. M., 123

Tang, A.
—; Shang, Z.; Teng, Q.; Pan, Y.; Cai, Z.; Zhao, X.; Feng, J.: Theoretical Study of the Structures and Electron Spectra of $C_{60}M_{12}$ (M = Li, Na, Be), 505
Teng, Q. See Tang, A., 505
Tomasi, J. See Rega, N., 219

Verkhivker, G. M. See Bouzida, D., 113
Verma, S. K. See Kumar, A., 307

Wang, N. See Lu, X., 377
Wang, Y.
—; Gunn, J. R.: Computational Study of Structures and Proton Transfer in Hydrogen-Bonded Ammonia Complexes Using Semiempirical Valence-Bond Approach, 357
Whitkop, P. G.
Integral Evaluation in the Case of a Helium Atom Positioned Off-Center in a Spherical Box, 459
Wijaywardene, M. See Nilsson, A. M., 85
Wilson, K. M. See Nilsson, A. M., 85
Winn, P. J. See Wu, P. H., 229
Wójcik, M. J.
—; Boczar, M.; Stoma, M.: Spectroscopic and Theoretical Study of Vibrational Spectra of Hydrogen-Bonded Tropolone, 275
Wu, J. H.
—; Winn, P. J.; Ferenczy, G. G.; Reynolds, C. A.: Solute Polarization and the Design of Cobalt Complexes as Redox-Active Therapeutic Agents, 229
Wu, T. See Chen, X.-Y., 417
Wu, Z. J.
—; Zhang, S. Y.: Calculation of Chemical Bond Parameters in $La_{1-x}Ca_xCrO_3$ ($0.0 \leq x \leq 0.3$), 433

Xin, X.-J. See Chen, J.-Q., 283
Xu, X. See Lu, X., 377

Yildiz, A. See Bulut, N., 425

Zaitsevskii, A.
—; Cimiraglia, R.: Diagrammatic Formulation of the Second-Order Many-Body Multipartitioning Perturbation Theory, 395
Zhang, Q. See Lu, X., 377
Zhang, S. Y. See Wu, Z. J., 433
Zhao, X. See Tang, A., 505
Zhikol, O. A. See Cheranovskii, V. O., 511

International Journal of Quantum Chemistry Subject Index—Volume 73

Ab initio, 1, 187, 209, 369
Ab initio calculations, 97, 317, 377, 417
Ab initio study, 161
Acylation mechanism, 161
Adrenergic receptors, 71
AlH($^1\Sigma$), 417
AMBER 4.1, 61
Ammonia, 357
Aromaticity, 451
Aspartate semialdehyde dehydrogenase, 137
Atomic coordinates, 439

Basis set, 307, 341
Basis set ab initio, 299
Basis set generating potential, 341
β-lactamases, 161
Binding energy landscapes, 113
Biological macromolecules, 219
Biomimetic models, 209
BSSE, 175
B3LYP/6-31G**, 349

C_{60}, 505
Canonical functions, 325
Cartesian Gaussians, 403
Catalysis, 137
$C_{20}H_{20}$, C_{80}, C_{240}, 283
CH_3 ClO, 29
CH_3OCl, 29
Chemical bond parameters, 433
Cluster modeling, 377
Cluster-surface analogy, 377
C—O bond breaking, 299
Computational chemistry, 1
Computer simulation, 249
Configuration interaction matrix elements, 23
Configuration state, 389
Confined quantum system, 459
Confined systems, 497
Continuum electrostatics, 45
Convergence, 333
Coordination compounds, 187
Core polarization potential, 403
Correlated mutation analysis, 85
Coupled differential equations, 479
Coupled Schrödinger equation, 325
CP corrections, 175
Crystal structure, 137
Crystalline state, 439
Cut-off function, 459
Cytochrome P450, 123

Density functional, 229
Density functional theory, 197, 299
Density functional theory (DFT), 369
DFT, 451
Dimers, 85
Dimethyl ether anion, 299
Dispersion contribution, 175
Docking, 71
Domain interfaces, 85

e vibrational mode, 369
Eigenvalue function, 325
Electron correlation problem, 395
Electrostatic potential, 71
Empirical valence bond method, 147
Enzyme, 137
Enzyme catalysis, 147
EPR, 249

Finite differences, 479
Fluctuating well-depth models, 469
Force-field parameters, 237
Fourier transform convolution theorem, 265
Free energy perturbation, 147
Fullerene molecule, 283

G proteins, 71
Galactose oxidase, 209
Gold–ethylene interaction, 317
Ground state, 511
GVB, 1

H_2 and HX elimination reactions, 37
HF molecule, 417
Heat of formation, 29
Helium atom, 459
Heme proteins, 249
High spin systems, 389
Homology modeling, 71, 97
H_2O_2, 249
Hydration, 229
Hydrogen bond, 357
Hydrogen-bonded tropolone, 275
Hydrogen clusters, 451

Impact parameter formalism, 307
Integral evaluation, 459
Intensity dependence of photodetachment rate, 469
Intermolecular interactions, 175

Jahn-Teller distortion, 505

Kinetic partitioning mechanism, 113
Kinetic stability, 37

$LA_{1-x}Ca_xCrO_3$, 433
Lanthanide chelates, 237
Ligand–protein docking, 113
Linear response, 45
Long-range interaction, 403
Low-Rydberg Na, 307

Magnesium oxide, 377
Magnetic properties, 451
Major histocompatibility receptor class II, 85
Many-body diagrams, 395
MCSCF, 1
Mechanism of action, 123
Methylenedioxyphenyl inhibitors, 123
MO calculations, 123
Model [NiFe] and [NiFeSe] hydrogenase active sites, 187
Model compounds, 187
Molecular dynamics, 45, 61, 71, 147, 209

Molecular dynamics simulation, 137
Molecular modeling, 237
Molecular recognition, 113
Molecular simulations, 237
Monte Carlo docking, 123
MRI, 237
Multireference perturbation theory, 395

N_8, 349
N_{10}, 349
N_{12}, 349
N_{14}, 349
N_{16}, 349
N_{20}, 349
N_{24}, 349
Ni–Fe hydrogenase, 197
ν_s stretching band, 275
Nuclear hormone receptors, 97
Numerical stability, 333

One-particle integrals, 403
Organometallic ferromagnets, 511
Overlap integrals, 333
Oxygen adsorption, 377

Parallel reaction channels, 417
Phase lag, 479
Phospholipic bilayer, 61
Photodetachment dynamics, photodetachment suppression by noise, 469
Poisson–Boltzmann, 229
Polarizable continuum model (PCM), 219
Polarization, 229
PPARγ agonists, 97
Protein interfaces, 85
Protein tyrosine phosphatase, 147
Proton transfer, 357
Pseudopotentials, 229, 317

Quantum chemistry, 1
Quartic oscillator, 497
Quasirelativistic effects, 317

Reaction dynamics, 425
Reaction probabilities, 425
Reactive scattering, 425

Scattering problems, 479
Schrödinger equation, 479
Semiempirical, 357
Semiempirical method, 433
SH_3X species, 37
Slater-type orbitals, 307
Slater-type orbitals (STOs), 333
Solvent effects, 219
Spatial confinement, 341, 497
Spectrum, 505
Spherical Laguerre Gaussian-type function (LGTF), 265
Spherical potential, 459
Spin-free permutation-group approaches, 23
Spin–orbit interactions, 23
Spin trap, 249
Stacking interactions, 175
Structure factor magnitudes, 439
Substituent effects, 37
Symmetry-adapted basis, 283

TDFGH method, 469
Theoretical chemistry, 439
Thermodynamics and Eyring transition state theory (TST), 417
Thiazolidinedione, 97
Translation, 333
Tree graph, 389
T-shaped interactions, 175
Two-electron integrals, 265

Uniform convergence, 403
Unitary shift operators, 23
Unrestricted dynamical density functional calculations, 209

Valence bond, 357
Variational method, 341
Vasopressin V2 receptor, 61
Vibrational spectra, 29, 275

Wave packet study, 425
Weighted histogram analysis method, 113
Weyl tableau, 389
WF_4 complex, 369
Wittig rearrangement, 299
WKB and MAF methods, 497